

Workflow 1 will help to find new potential indications and score them for known drug using Pathway Studio. It start from particular drug and it's main targets.

Workflow 2 start from particular disease including rare disease, seek known targets for the disease using Pathway Studio. As a next step Reaxys Medicinal Chemistry will help to find all inhibitors targets found. The molucelas would be filtered to have appropriate affinity to the targets, to pass at least I phase of clinical trails, to have $Mw \leq 400$, $LogP \leq 5$, Hydrogen bond donor ≤ 3 , Hydrogen bond acceptor ≤ 7 . Additional information about action of molecules would be collected using Pathway Studio. Example of the results is shown on figure 1.

Figure 1. Humira indications reported in clinical trials and biomedical literature as found in Pathway Studio database and annotated in Pathway Studio interface

